

Accepted Manuscript

Structural and elastic DFT study of four structures for $\text{Cu}_2\text{ZnSnS}_4$ under high pressure

Yifen Zhao, Decong Li, Zuming Liu



PII: S0925-8388(16)33559-9

DOI: [10.1016/j.jallcom.2016.11.091](https://doi.org/10.1016/j.jallcom.2016.11.091)

Reference: JALCOM 39587

To appear in: *Journal of Alloys and Compounds*

Received Date: 21 July 2016

Revised Date: 6 November 2016

Accepted Date: 7 November 2016

Please cite this article as: Y. Zhao, D. Li, Z. Liu, Structural and elastic DFT study of four structures for $\text{Cu}_2\text{ZnSnS}_4$ under high pressure, *Journal of Alloys and Compounds* (2016), doi: 10.1016/j.jallcom.2016.11.091.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Structural and elastic DFT study of four structures for $\text{Cu}_2\text{ZnSnS}_4$ under high pressure**Yifen Zhao¹, Decong Li², Zuming Liu^{1*}**

¹*Education Ministry Key Laboratory of Renewable Energy Advanced Materials and Manufacturing Technology, key Laboratory of Rural Energy Engineering in Yunnan Province, Solar Energy Research Institute, Yunnan Normal University, Kunming, Yunnan Province, 650500, People's Republic of China*

²*College of Optoelectronic Engineering, Yunnan Open University, Kunming, Yunnan Province, 650223, People's Republic of China*

Abstract

We have systematically investigated the structural and elastic properties of the zincblende-derived and wurtzite-derived structures of $\text{Cu}_2\text{ZnSnS}_4$ (CZTS) under various pressures utilizing first principles calculations within density functional theory (DFT). The results revealed that the enthalpy-pressure curves of kesterite (KS) and stannite (ST) intersect at approximately 32 GPa, while the curves of wurtzite kesterite (WKS) and wurtzite stannite (WST) phases intersect at approximately 52 GPa, which suggests that the phase transitions or mixed crystals occur in the WKS and WST structures. Furthermore, in the KS and ST structures, shear modulus (G) and Young's modulus (E) decrease with an increase in pressure, which indicates that stiffness reduces with increasing pressure. However, in the WKS and WST phases, G and E first decrease and then increase with an increase in pressure. Moreover, owing to Pugh's ductility index (G_H/B_H) being less than 0.57, all four CZTS structures are ductile in nature under different pressures. In the KS and ST phases, Poisson's ratios (γ) increase gradually, when the pressure increases. Whereas, in the WKS and WST structures, the Poisson's ratios (γ) are greater than the Poisson's ratios (γ) under the zero pressure, which indicates better plasticity. Furthermore, it is

*Corresponding author. E-mail address: zmluipv@126.com

Download English Version:

<https://daneshyari.com/en/article/5461273>

Download Persian Version:

<https://daneshyari.com/article/5461273>

[Daneshyari.com](https://daneshyari.com)